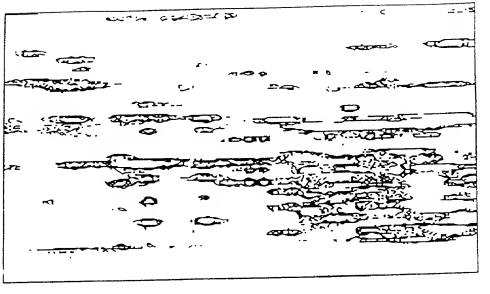
FIGURE 1A

A



09932820.102201

FIGURE 1B

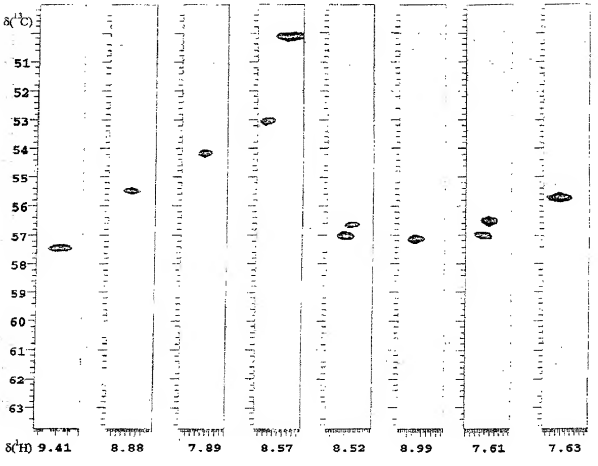


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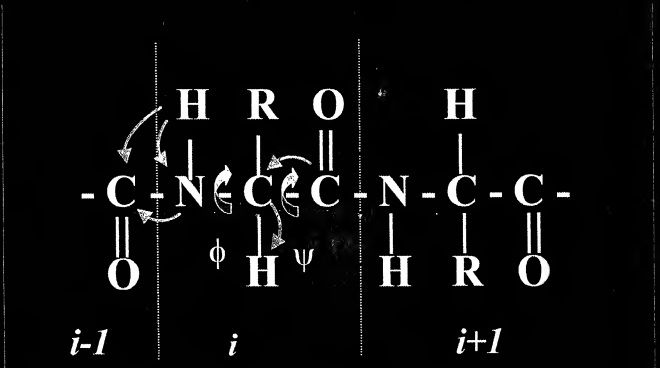
FIGURE 2

B

Dipolar Couplings That Depend Only on ϕ(i) and ψ(i)



Search ϕ and ψ Until Measured Couplings = Theoretical Couplings

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Packing Secondary Structural Elements

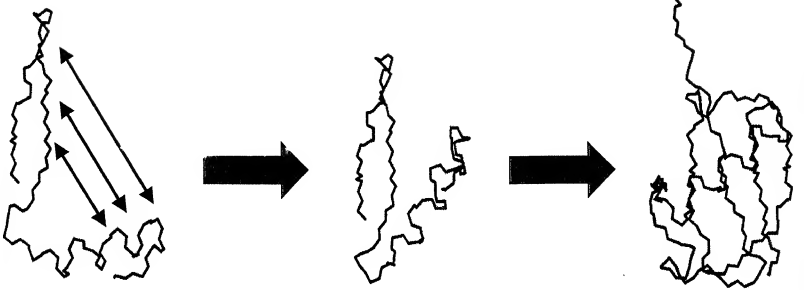
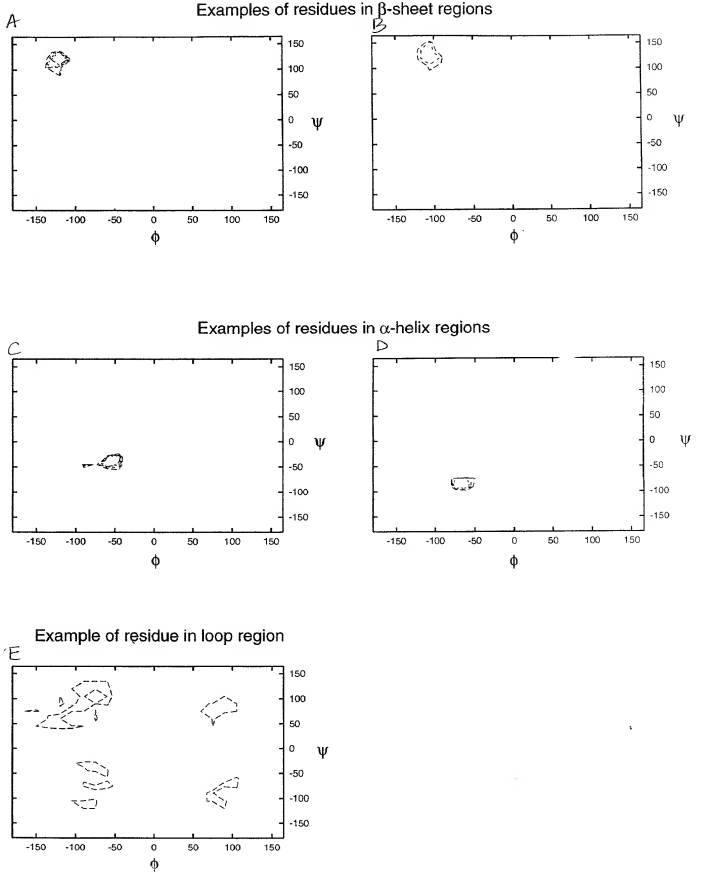


FIGURE 4



10220147.020199

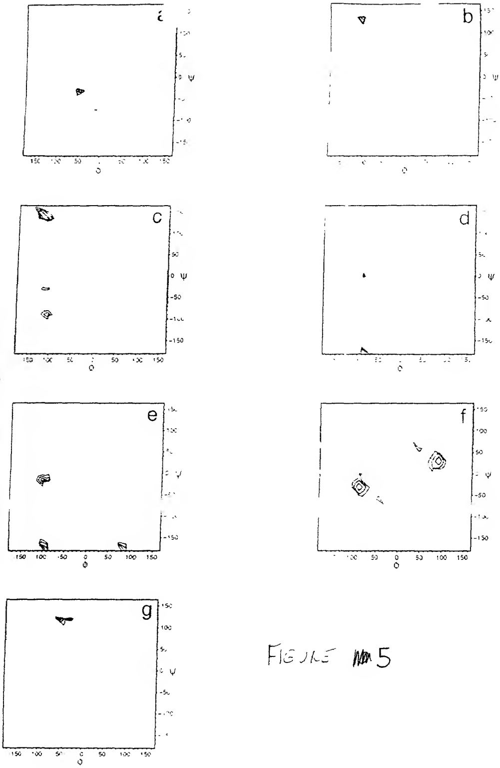


FIGURE 5

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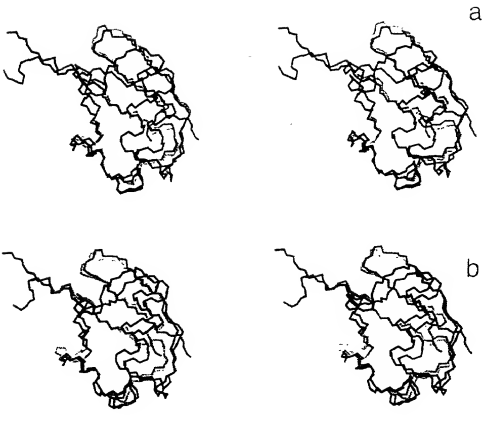

FIGURE 6

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FIGURE 7

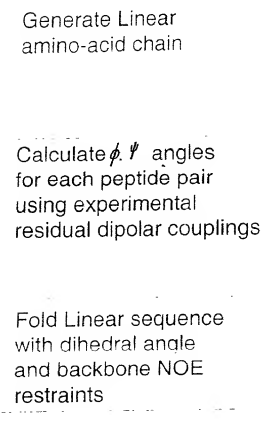

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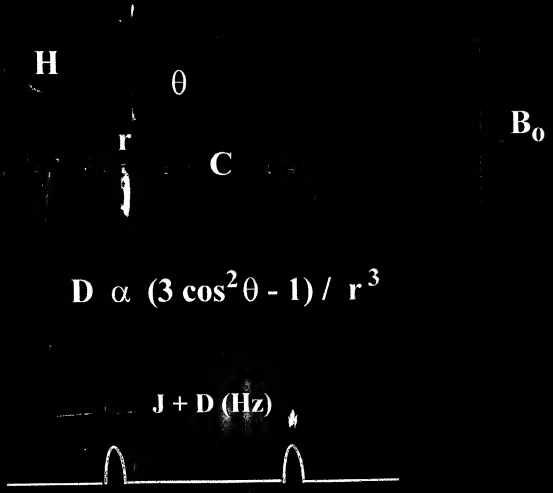
FIGURE 8

Dipolar Couplings - Powerful Structural Constraints



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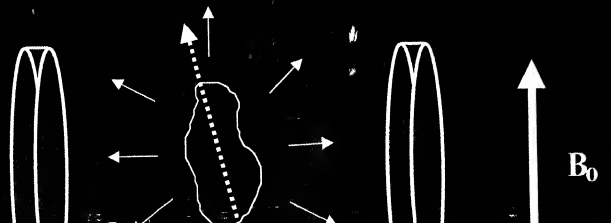
Measurement of Dipolar Couplings Requires a Weakly Aligned Molecule



Phospholipid Bicelles

22° C: Isotropic (no alignment)

J (Hz)

35° C: LC Phase (alignment)

J + D (Hz)

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FIGURE 10

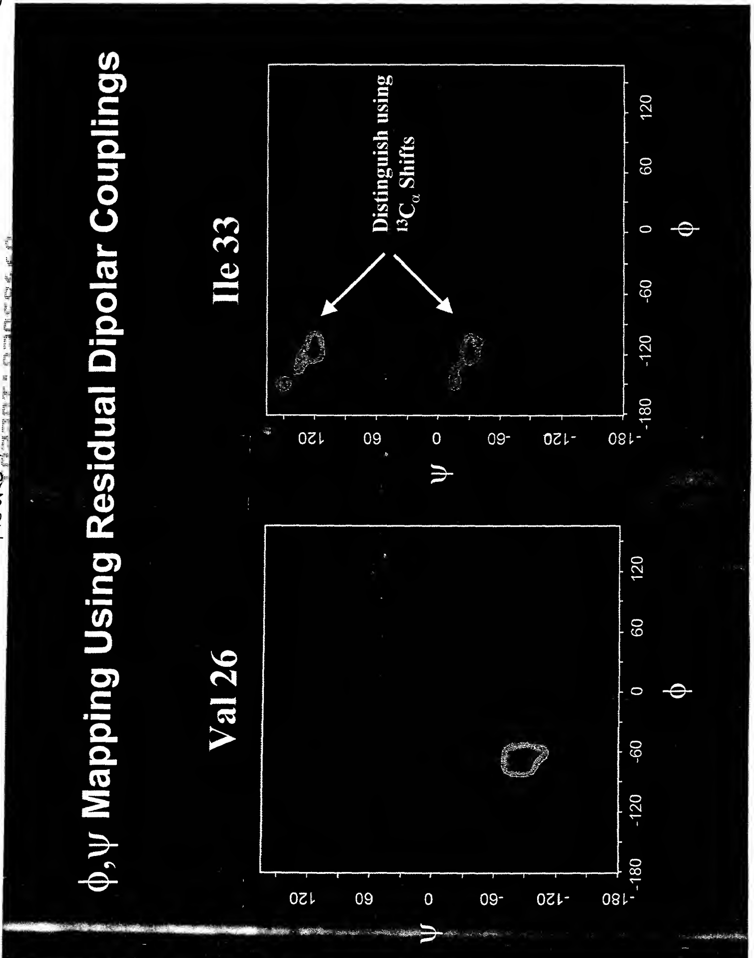
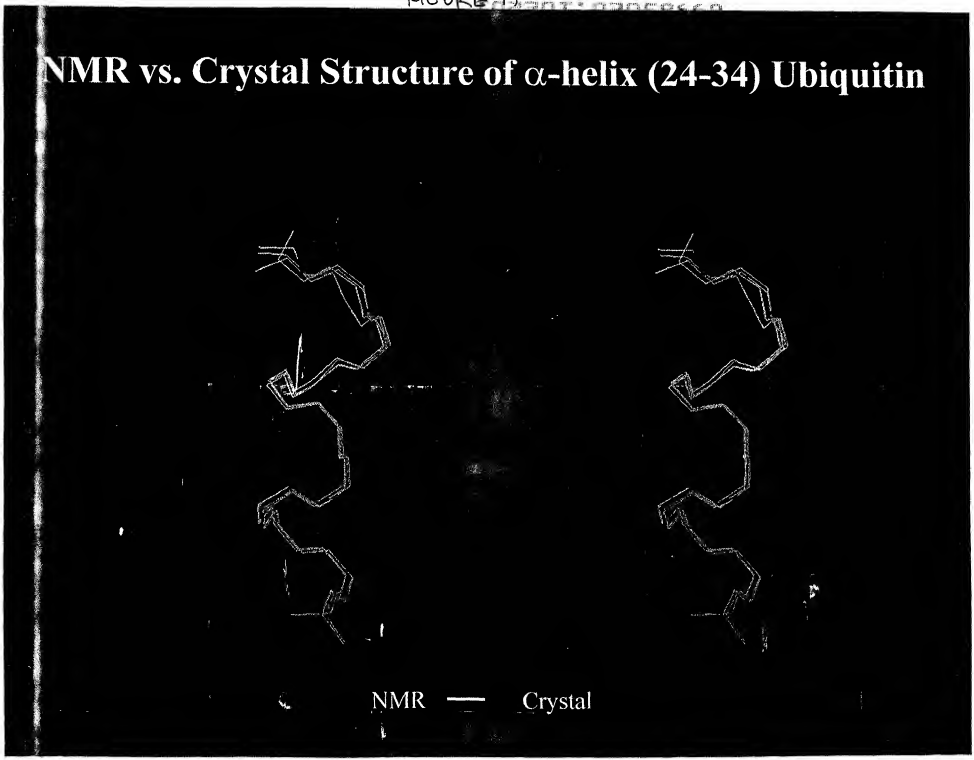

φ,ψ Mapping Using Residual Dipolar Couplings
Val 26
Ile 33
Distinguish using
$^{13}C_{\alpha}$ Shifts
φ
ψ
-180
-120
-60
0
60
120

FIGURE 11


NMR vs. Crystal Structure of α-helix (24-34) Ubiquitin
NMR
Crystal

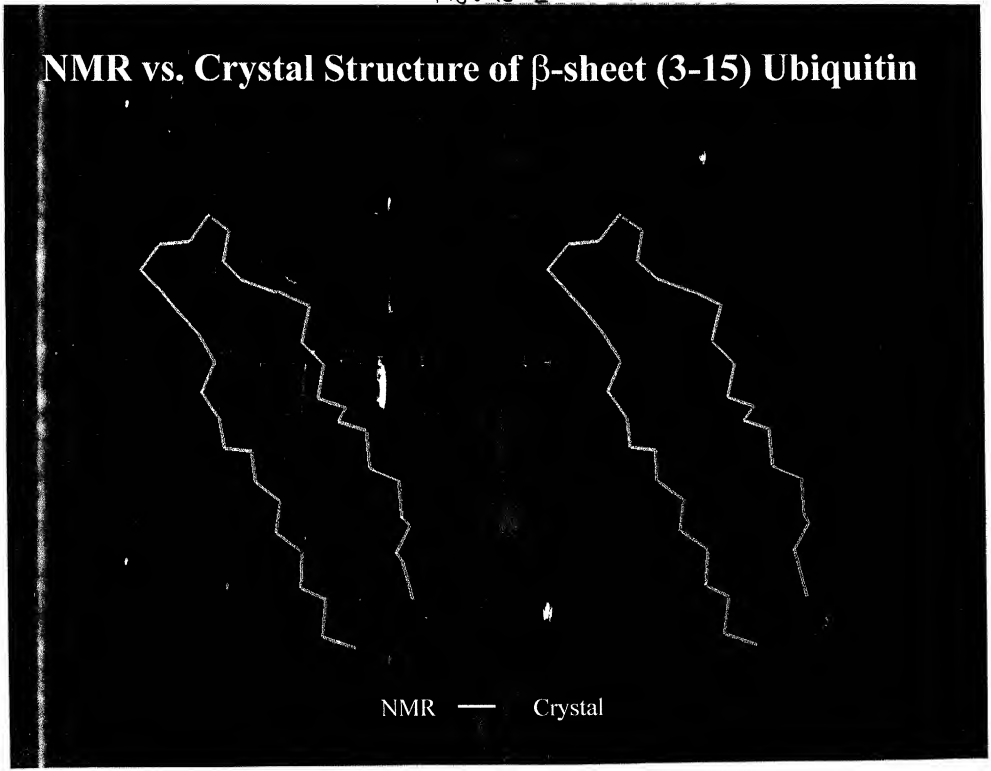
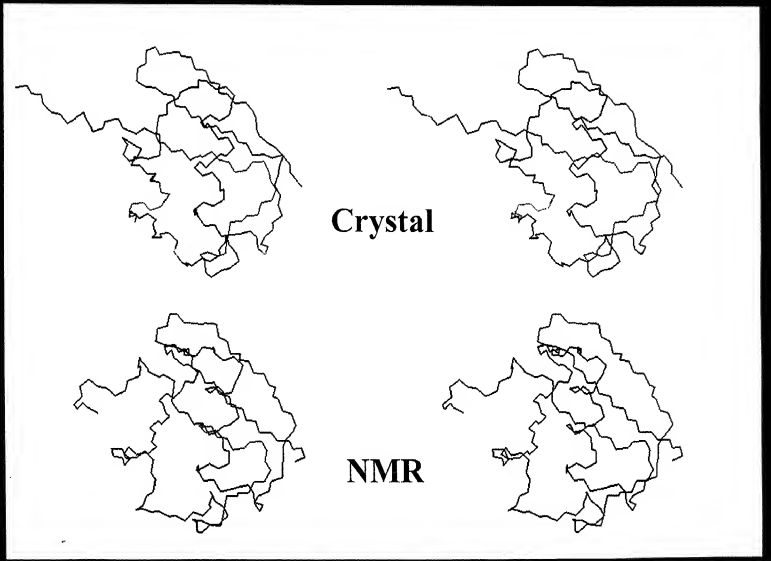

NMR vs. Crystal Structure of β-sheet (3-15) Ubiquitin
NMR
Crystal

FIGURE 13

Crystal Structure vs. NMR Global Fold - Ubiquitin



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